

Jump Events in a 3D Edwards-Anderson Spin Glass

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The statistical properties of infrequent particle displacements, greater than a certain distance, is known as jump dynamics in the context of structural glass formers. We generalize the concept of jump to the case of a spin glass, by dividing the system in small boxes, and considering infrequent cooperative spin flips in each box. We perform numerical simulations for the Edwards-Anderson 3D model, and study how the properties of these jumps depend on the waiting time after a quench. Similarly to the results for structural glasses, we find that while jump frequency depends strongly on time, jump duration and jump length are roughly stationary. For short enough times, the rest time between jumps is approximately constant. For longer times, it varies as the inverse of jump frequency, and cannot be considered an independent property of jumps.

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I. INTRODUCTION

Glass formers and spin glasses have been the subject of intense theoretical, experimental and numerical research in the last decades (see for instance, [1–3] and references therein). These systems present similar phenomenology (see for instance [4]), analogous techniques have been developed in both [5, 6], and their relationship has been proved [7–9]. Thus, in spite of the details about composition, structure or kind of degrees of freedom, it is common to use the word *glassy* to refer to any material with a dynamics qualitatively similar to that of a glass [10].

The study of glassy systems poses a series of issues, related to the impossibility to reach equilibrium below the glass transition temperature T_g . In this case, the system evolves for ever. However, the time dependence of the one-time observables, like density, energy, pressure or magnetization (in a magnetic system) is quite weak and hard to appreciate. *Aging* effects are more clearly observed in the behavior of two-time observables, like the autocorrelation $C(t_2, t_1)$ and response $R(t_2, t_1)$ functions, which do not depend only on the time difference $t_2 - t_1$ but on t_1 and t_2 (see, for example, [11–13]).

An alternative is to study *aging-to-equilibrium* [14, 15], based in the idea that, if a system is quenched from an equilibrium state at a temperature T_0 to a lower temperature $T_F > T_g$, the transition to equilibrium takes place on a time scale related to the equilibrium relaxation time $\tau(T_F)$, and it will show some aspects of glassy dynamics for $t \ll \tau(T_F)$. In [15], two-time correlation functions were studied in both aging-to-equilibrium and aging regimes for a simple glass former. In [14], the authors analyzed the aging-to-equilibrium dynamics for the strong glass former SiO_2 .

Most of the studies about glassy systems focus on *macroscopic* or global observables. Nevertheless, in recent years *microscopic* (i. e., involving a single or few particle) actions have been analyzed [16–20] in structural glass formers, with the goal of understanding better the mechanisms responsible for aging. In [16], the microscopic dynamics of SiO_2 were analyzed and related to the macroscopic dynamics. After a quench, *jump* events, i. e., particle movements greater than a certain threshold, were detected and their statistical properties were analyzed. The authors found that the number of jumping particles decreases strongly with t , the time elapsed since the quench, reaching equilibrium at times compatible with $\tau(T_F)$. Interestingly, jumps themselves (average length, time duration, and even rest time between consecutive jumps) do not depend on t .

Jump events are not only closely related to macroscopic evolution observables like diffusivity [21] but constitute an important ingredient in the relaxation of glass formers. They provide a link among structure and dynamics, by giving a more quantitative idea of the *cage* effect. This is the case in [22], where, for a 2D model at low temperature, it is found that non jumping particles were more likely in highly ordered environments. The relationship among jumps and dynamical heterogeneities has also been established [23].

In this work, we study some microscopic aspects of the aging-to-equilibrium and aging dynamics of the well known 3D Edwards-Anderson (EA) spin-glass model [24–26]. This model has been extensively studied in a macroscopic way. Some microscopic results have also been reported [27], including the existence of a backbone [28].

We start by generalizing the concept of jump, introduced originally for structural glass formers [16], to the case of a spin glass. We wish to analyze whether the above mentioned statistical properties of jump events can be reproduced in a glassy system composed of spins, instead of moving particles.

For the EA model, we find that microscopic and macro-

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scopic relaxation times behave similarly. We also find that some variables depend strongly on time while others are nearly stationary. Thus, most of the results in [16] for a structural glass former hold for this spin glass model. For instance, jump length and jump duration are roughly stationary, while the number of jumps depends strongly on t . On the other hand, we find that rest time between jumps, which is independent of time in [16], has an inverse relation to jump frequency for the EA model. We draw a plausible explanation for this discrepancy.

The paper is organized as follows. In Sec. II, we describe the model and observables. In Sec. III, we define an equilibration time based on macroscopic observables. Main results, i.e., evolution of microscopic observables, are presented in Sec. IV. In Sec. V, we draw our conclusions.

II. MODEL AND OBSERVABLES

We study the Gaussian EA model in a cube with L spins by side, under periodic boundary conditions, defined by the Hamiltonian:

$$H = - \sum_{\langle i,j \rangle} J_{ij} S_i S_j,$$

where the indexes i, j run from 1 to L^3 . Spin variables take values $S_i = \pm 1$ and the pairs $\langle i, j \rangle$ identify nearest-neighbors. The couplings are taken randomly with a Gaussian distribution with zero mean and unit variance.

Dynamics is simulated with Metropolis algorithm. That is, at each Monte Carlo (MC) step, $N = L^3$ spin flip trials are performed. They are accepted or rejected according to their Boltzmann weights.

For this system, $T_g \simeq 0.92$ [29]. So, in order to study aging-to-equilibrium, and also aging-to-non-equilibrium, we equilibrate the system at temperature $T_0 = 3$ (we have also performed runs for $T_0 = \infty$) for 10^5 MC steps. We define $t = 0$ as the time at which the system is quenched to the final temperature $T_f = 1.5, 1.2, 1.0$ and also 0.9 which is below T_g . We have run 640 samples for each temperature, for 10^6 MC steps, or more, after the quench.

In next paragraphs, we define several microscopic observables, by dividing the full system into cubic boxes of side l_b , which contain $N_b = l_b^3$ spins each. Unless explicitly stated, we have worked with $L = 16$ and $l_b = 4$. Then, each box C_i is labeled with index i running from 1 to 64. We record the configuration every $\delta t = 5$ MC steps which we will call a unit time.

We define the overlap between consecutive records of box i as

$$O_i(t) = \frac{1}{N_b} \sum_{j \in C_i} S_j(t) S_j(t - \delta t), \quad (1)$$

which we compute for $t = n\delta t$, with n a positive integer.

We also compute the magnetization M_i and the energy E_i of every box.

$$M_i(t) = \sum_{j \in C_i} S_j(t) \quad (2)$$

$$E_i(t) = \frac{1}{2} \sum_{j \in C_i, k} J_{jk} S_j(t) S_k(t), \quad (3)$$

where k is a nearest neighbor of j .

When the simulation ends, we calculate $\langle O_i \rangle$ and $\langle O_i^2 \rangle$, for all boxes averaged in the time window $5 \cdot 10^5 \text{ MC} < t < 10^6 \text{ MC}$. With this, we calculate $\sigma_i = \sqrt{\langle O_i^2 \rangle - \langle O_i \rangle^2}$. In Fig. 1 we show the values of O_i and σ_i averaged over small time windows of 10000 MC steps, for a single box ($i = 1$). We see that both quantities are nearly constant even for the lowest temperature $T = 0.9 < T_g$. This makes them reasonably robust parameters to study jumps.

Greater changes in the configuration of a single box are related to smaller values of the overlap between two consecutive configurations. We will say that box i is jumping at time t if

$$O_i(t) < \langle O_i \rangle - \gamma \sigma_i. \quad (4)$$

We have taken $\gamma = 3$ in most of the cases, although we have also studied $\gamma = 5$. The jump starts at t_i , where t_i is the greatest value that verifies both $t_i < t$ and that Eq. (4) does not hold for t_i (i.e. $O_i(t_i) \geq \langle O_i \rangle - \gamma \sigma_i$). Similarly, the jump ends at $t_f > t$, if $t_f + \delta t$ is the smallest value that does not verify Eq. (4).

We define the *jump frequency* ν , as the number of jumps per box per unit time. We measure it as a function of t . For each jump we define a *jump duration* as $d = t_f - t_i$. We define the *rest time* r , as the time the particle waits until next jump. That is, the difference between t_i for the next jump and t_f for the current jump. We define the *jump size*, l , using overlap values: we calculate the sum of the overlap changes over the times belonging to the jump, i.e. $l = \sum_{t_i < t \leq t_f} N_b - O_i(t)$.

We also compute some macroscopic one-time quantities as the total energy, magnetization, and number of spins that flip, and the global two-time correlation $C(t + \Delta t, t)$:

$$C(t + \Delta t, t) = \frac{1}{N} \sum_{i=1}^N S_i(t) S_i(t + \Delta t). \quad (5)$$

III. RESULTS: MACROSCOPIC QUANTITIES

We want to measure the time it takes to equilibrate the system, using a macroscopic variable. It would be desirable to find τ_e^{ideal} such that for $t > \tau_e^{\text{ideal}}$, $C(t + \Delta t, t)$ does not depend on t . We cannot do that due to limited precision in our data. Following [15], we define

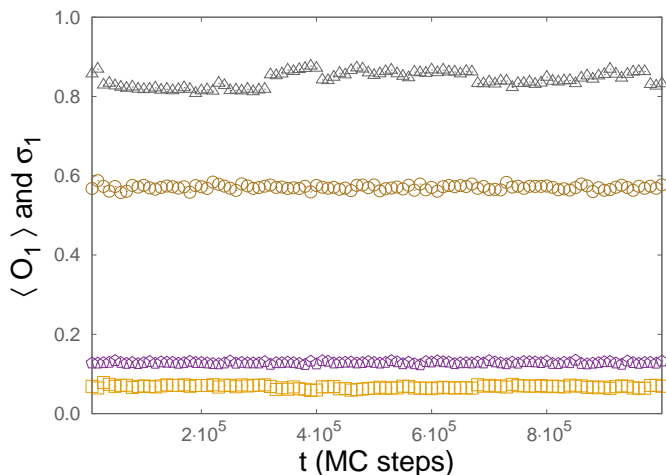


FIG. 1. (Color online) σ_1 and $\langle O_1 \rangle$ for a single box as a function of t for different temperatures. Black triangles: $\langle O_1 \rangle$ for $T_F = 0.9$. Grey spheres: $\langle O_1 \rangle$ for $T_F = 1.5$. Orange squares: σ_1 for $T_F = 0.9$. Violet pentagons: σ_1 for $T_F = 1.5$.

an auxiliary variable $\tau_a(t)$ such that $C(t + \tau_a(t), t) = K$. In our case, we choose $K = 0.2$.

In Fig. 2-top, we show the two-time correlation as a function of t for various t for temperature $T = 1.5$. In Fig. 2-bottom, we plot $\tau_a(t)$ for $T = 1.5$. For $T_F > T_g$, the relaxation time is then $\tau_a^{EQ}(T_F) = \lim_{t \rightarrow \infty} \tau_a(t)$. From Fig. 2-bottom, we see that $\tau_a(t)$ grows with t until it gets a constant value. We have fitted $\tau_a(t)$ with $(C_1 + C_2 \cdot \log(t)) e^{-t/C_3} + C_4 \cdot (1 - e^{-t/C_3})$. From this fit, we can define $\tau_e = C_3$. Using this procedure, we were able to get τ_e for $T = 1.5, 1.35$ and $T = 1.2$. Although $T = 1.0 > T_g$ we were unable to estimate τ_e for this temperature, since it exceeds our simulation time.

We have checked, for $T_F \geq 1.2$, that τ_e is a good estimate of the macroscopic equilibration time for the one-time macroscopic variables, like total energy and number of flips.

IV. RESULTS: MICROSCOPIC QUANTITIES

We analyze the time evolution of the statistical properties of jump events after a quench.

In Fig. 3, we show the jump frequency as a function of time in logarithmic scale. We have added data for $T_0 = \infty$ and $T_F = 1.0$, which looks qualitatively similar, at least with our time windows, as data for $T_0 = 3$. This result holds for other values of T_F (not shown). We see a steep decrease, consistent with the results of [16]. The slope is greater for lower temperatures and time for which the decreasing of ν becomes negligible are compatible with macroscopic relaxation times for temperatures $T_F \geq 1.2$, where we are able to measure τ_e . We have indicated these values with arrows at the bottom of Fig. 3, to facilitate comparison.

In Fig. 4, we plot both jump duration and rest time

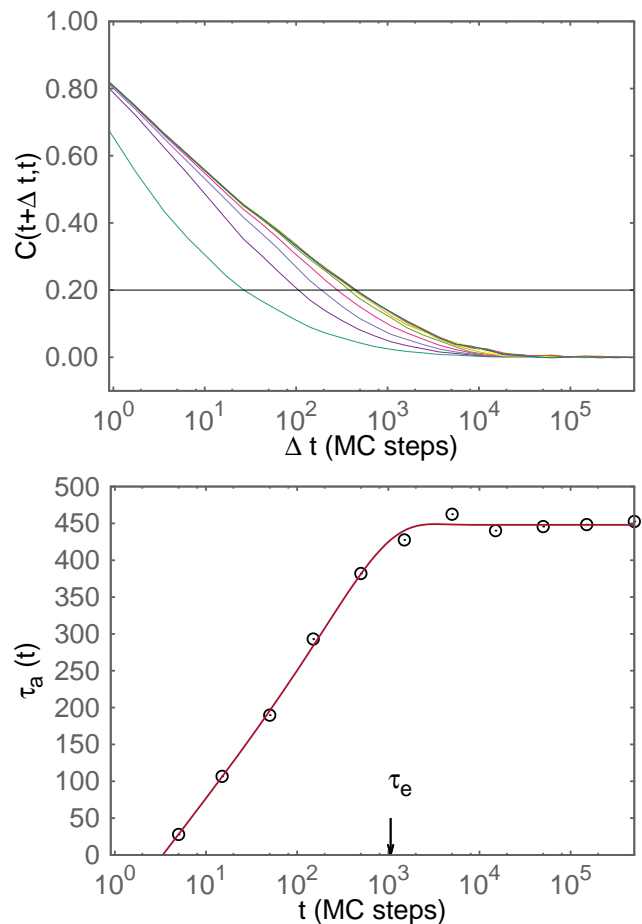


FIG. 2. (Color online) Top: Global two-time correlations for $T_F = 1.5$, and several waiting times. From left to right, $t = 5, 15, 50, 150, 500, 1500, 5000, 15000, 50000, 150000, 500000$ MC steps. The horizontal line corresponds to $C(t + \Delta t, t) = 0.2$. The arrows indicate $\tau_a(t)$ for each t . Bottom: τ_a as a function of t for $T_F = 1.5$ (black circles). The (red) line corresponds to the fitting function $(C_1 + C_2 \log(t)) e^{-t/C_3} + C_4 (1 - e^{-t/C_3})$. The arrow indicates $\tau_e = C_3$.

against time. It is apparent that the first is of the order of δt , which means that most of the jump last one unit time. This is similar to what reported in [16], where average jump duration is close to time step. Jump duration decreases very slowly with temperature and has no appreciable time dependence even before τ_e . However, at odds with [16], rest time seems to evolve with t . This will be further discussed in next subsection.

In Fig. 5, we show the average value jump size. Note that this quantity stabilizes before equilibration time. Even for $T = 0.9$, which is below T_g , it does for $t \sim 10^4$.

To summarize, at all temperatures, some variables change in a much more pronounced way than others. This can be better appreciated in Fig. 6, where we show all the previous data for $T = 1.0$ in logarithmic scale. Results are shifted (multiplied by a constant) to facilitate comparison. Let us remark that while the number of

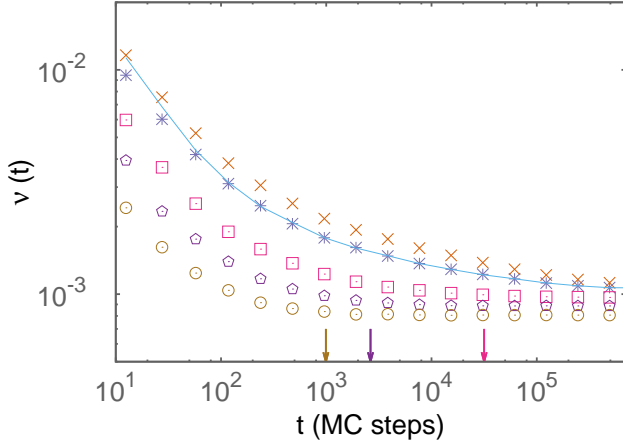


FIG. 3. (Color online) Jump frequency as a function of time. Symbols correspond to $T_0 = 3$, from top to bottom, $T_F = 0.9$, 1.0, 1.2, 1.35 and 1.5. Line with no symbols is for $T_0 = \infty$, $T_F = 1.0$. Arrows showing τ_e for $T_F = 1.5$, 1.35, and 1.2 (from left to right) have been added at figure bottom.

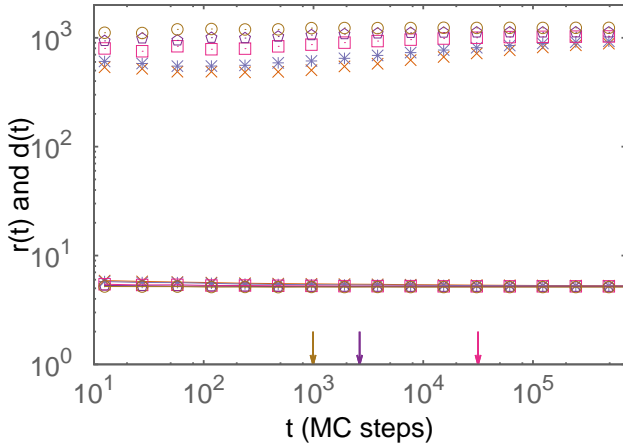


FIG. 4. (Color online) Rest time (symbols) and jump duration (lines with symbols) as a function of time. For $t > 10^5$ there is an artificial decrease of rest time, related to the finite simulation time. Symbols and colors are the same as in Fig. 3. Results for $T_0 = \infty$ were avoided for the sake of clarity.

jumps decreases by about one order of magnitude, other variables have negligible changes (as in [16]), with the only exception of rest time, which grows at long times.

A. Issues with rest time

In Ref. [16], the authors study jumping particles, while in this work we study jumps of boxes. These quantities behave similarly, however we have found a discrepancy in the behavior of the rest time; which is roughly constant in [16]. Since, according to our simulations (see, for example, Fig. 4), there exist time dependence for this quantity, some words are in order.

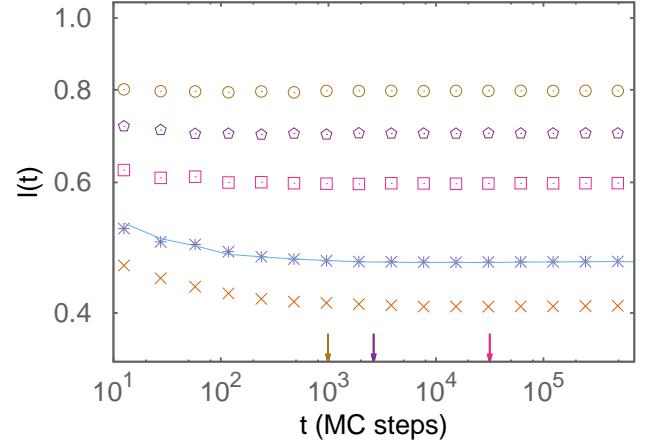


FIG. 5. (Color online) Jump size as a function of time for several temperatures. Symbols and colors are the same as in Fig. 3.

	T_F		
	0.9	1.0	1.2
s_ν	-0.082 ± 0.005	-0.054 ± 0.004	-0.013 ± 0.002
s_r	0.080 ± 0.005	0.053 ± 0.004	0.013 ± 0.002

TABLE I. Long-time effective exponents for jump frequency and rest time for $\gamma = 3$ (for higher temperature, the average exponents are smaller than their errors). In all cases, data were fitted in the range $10^4 < t < 5 \cdot 10^5$.

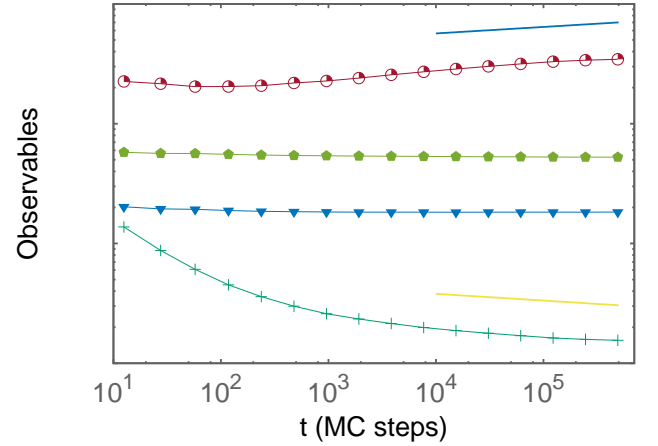


FIG. 6. Results for all observables for $T = 1.0$, shifted so that comparison becomes more clear. From top to bottom: rest time (Purple quarter filled circles); jump duration (Green pentagons) Jump size (Blue triangles), and jump frequency (Dark green crosses). Straight lines are the fit of jump frequency and rest time as a function of t , using power-law forms in the range $10^4 < t < 5 \cdot 10^5$. Fitted slopes are shown in table I.

For short enough times, i. e., for $t \ll \langle r \rangle$, most of boxes jump once or never. The results corresponding to $r(t)$ in Fig. 4 indicate that in this time interval ($\langle t \rangle \simeq 10^3$ MC

steps) jump duration is nearly constant. For longer times ($t \gg \langle r \rangle$), when most of jumping boxes do many jumps, it should exist some correlation between rest time and jump frequency. Since jump duration is much smaller than time between jumps, the average number of jumps per unit time, multiplied by the rest time, should be equal to the total time multiplied the number of boxes, i. e., $r\nu \simeq 1$. Thus, for long enough times, we expect that r increases as ν decreases. Notice that this is what happens in Fig. 6, where the long-time effective exponents for jump frequency ($\nu(t) \sim t^{s_\nu}$) and rest time ($r(t) \sim t^{s_r}$) are opposite ($s_\nu \simeq -s_r$) within statistical error. The same happens for other temperatures, see table I.

B. Sensitivity of results

In this subsection we present the results of several tests we carried out to analyze the robustness of the statistical properties of jump events.

We have checked that the outcomes for $T_0 = 3$ are similar to those for $T_0 = \infty$. Thus, most interesting results do not depend much on T_0 . We have also verified that doubling system size (working with a system of size $L = 32$) does not change the results within statistical error. Also, we found qualitatively the same results for different unit times $\delta t = 2, 5$ and 100, though choosing smaller δt makes the decreasing of ν more pronounced.

Using an alternative definition of jumps, by changing the value of γ , also leads to the same qualitative behavior. For instance, a higher γ (more restrictive definition, then fewer jumps) makes effective exponent of ν more negative. For example, we can compare the results for $\gamma = 5$, shown in Fig. 7, with those for $\gamma = 3$, in Fig. 6. Notice that, in first case, ν decreases by two orders of magnitude, while it decreases about one order of magnitude for the second. On the other hand, we can observe that in Fig. 7 the rest time remains nearly constant for a longer period of time than in Fig. 6. The reason for this behavior is that, for $\gamma = 5$ the average of the rest time $\langle r \rangle$ is of the order of 10^5 (while $\langle r \rangle \simeq 10^3$ for $\gamma = 3$). In addition, as $\langle r \rangle$ is close to the total simulation time, it is impossible to evaluate the rest time of most jumps that happen at $t \gtrsim 10^5$. Thus, the largest values of rest times are neglected, and r becomes underestimated. As a consequence, the effective exponents leading ν and r for $\gamma = 5$, have values with opposite signs but not exactly the same absolute value ($s_\nu = -0.128 \pm 0.009$ and $s_r = 0.0767 \pm 0.011$). For $\gamma = 7$, the proportion of neglected rest times is even greater, and we get both s_ν and s_r negative.

We have also studied *jump energy* and *jump magnetization*, defined as the absolute value of the energy and magnetization differences of each box before and after the jump. These variables do not sensitively evolve with t . The energy and magnetization of every box also become stationary well before τ_e . Varying γ , we found that less frequent jumps are related to greater changes in magne-

tization and energy.

We have explored the use of an alternative criteria of jump, with the same threshold for every box. That is, by considering that box i is jumping at t when $O_i(t) < B$, with the same constant B for all boxes. We find that, since every box has a different quenched disorder, we get *fast* boxes jumping very frequently and *slow* boxes, jumping few times in the simulation time. So this definition gives some unwanted results; related to the fact that rest time is severely underestimated at long t .

Finally, we have tried other jump criteria by defining a jump when magnetization differences overcome a certain threshold. We have found similar results to the ones presented here using this alternative criteria.

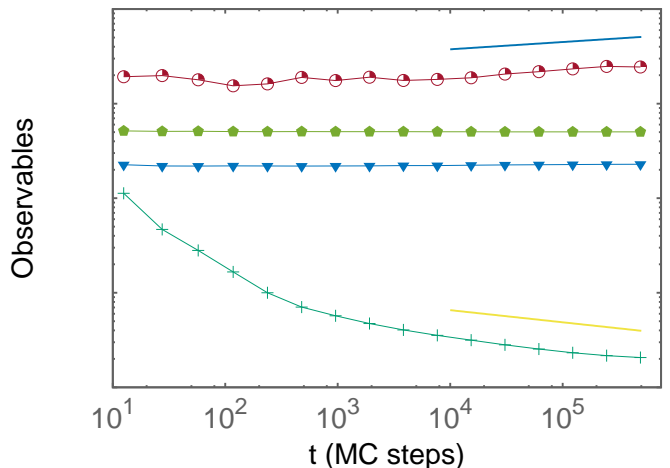


FIG. 7. (Color online) Time evolution of jump properties for $\gamma = 5$. From top to bottom: rest time, jump duration, jump size, and jump frequency. Sets of data points are shifted vertically to facilitate comparison. Let us remark that $\langle r \rangle \simeq 10^5$, which explains why the absolute values of $s_\nu = -0.128 \pm 0.009$ and $s_r = 0.0767 \pm 0.011$ (indicated with straight lines) do not coincide.

The results of these tests give support to the idea that, in spite of the manner we define a jump, we always get a jump frequency which depends strongly on time, but jump properties (with the exception of r , at long times) reach stationarity much before the equilibration time.

V. CONCLUSION

In this work, we generalize the concept of jump, introduced in the context of glass formers [16], to the case of spin glasses. We divide the system into boxes, and define a jump as a cooperative spin flipping making the overlap function of a box to decay below a certain amount in a small time interval δt .

We study the statistical properties of these jumps as a function of the waiting time t after a quench, for a Edwards-Anderson 3D model of spin glass.

When this system is quenched to a temperature T_F higher than the glass transition temperature $T_g \simeq 0.92$, it reaches equilibrium after a characteristic time τ_e , which we determine numerically from the stabilization of the global two-time correlation function $C(t + \Delta t, t)$. We confirm that every statistical property of jumps becomes independent of time for $t > \tau_e$. Interestingly however, in the dynamics of relaxation towards equilibrium, we find that most one-time microscopic observables related to jumps become nearly stationary well before τ_e , similarly to what reported for structural glass formers [16]. The exception being the jump frequency, which is a clearly decreasing quantity for times much closer to the equilibration time; $t \lesssim \tau_e$. Let us mention that even if at long enough times rest time is a growing observable, it evolves inversely to jump frequency, and, in this sense, it is not an independent quantity. For $T_F < T_g$, when the equilibration time diverges, we observe that all the measured microscopic observables depend on time, in the time interval that corresponds to our simulations. However, while jump duration and jump size change very slowly, jump frequency decreases much faster. This sug-

gests that in the glass phase the number of jumps always decreases but jumps themselves are not t sensitive at long times.

These conclusions do not depend qualitatively on the chosen values of δt , system size, box size nor the details of the criteria to define a jump. In particular, if jumps are defined as a function of magnetization or energy changes instead of overlap changes, similar results are found.

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